

Organic Semiconductor Light-emitting Diodes for Solid State Lighting

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The object of solid state lighting is to replace conventional incandescent and fluorescent light bulbs with highly efficient solid state light-emitting diodes (LEDs). Lighting is an extremely large business that consumes about one quarter of the electricity produced annually in the United States. Over 10^{18} J (about 300 Megatons of TNT) of energy are expended for lighting annually. Efficient semiconductor LEDs have the potential to replace both fluorescent and incandescent lights as the primary lighting source. They are potentially more efficient and more environmentally benign (no Hg) than these current lighting sources. In addition, semiconductor LEDs have unique properties that make them attractive for lighting applications—it is possible to electrically control the spectral properties of the light emitted, and they can be arranged over large areas in various shapes for aesthetic purposes.

There are two basic kinds of semiconductor LEDs being explored for solid state lighting: inorganic semiconductor LEDs, and organic semiconductor LEDs. Inorganic semiconductor LEDs use crystalline materials like GaN and organic semiconductor LEDs use disordered materials based on conjugated hydrocarbons (i.e., materials with double carbon-carbon bonds), like the polymer poly-phenylene vinylene (PPV). Inorganic semiconductor LEDs make bright point light sources. Figure 1 shows a set of inorganic semiconductor white LEDs used for solid state lighting. Organic semiconductor LEDs make large area light sources. Figure 2 shows a white organic LED illuminating a color chart. At present inorganic LEDs are somewhat further developed than organic LEDs for solid state lighting applications.

At Los Alamos we are involved in the investigation of organic semiconductors for a variety of applications including organic LEDs for solid state lighting. The basic device structure of an organic LED is shown in Fig. 3. It consists of a thin (typically about 100 nm) layer of organic semiconductor sandwiched between two conducting contacts. The organic semiconductor is undoped and highly resistive. Electrons are injected into the organic semiconductor from one of the conducting contacts and holes are injected into the organic semiconductor from



Fig. 1. Inorganic semiconductor white LEDs for solid state lighting.

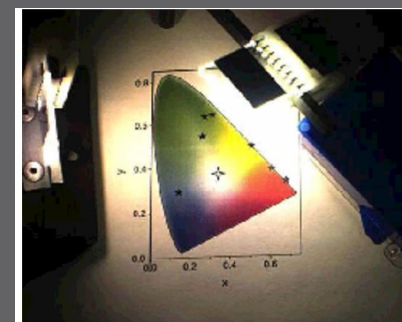


Fig. 2. Organic semiconductor white LEDs for solid state lighting.

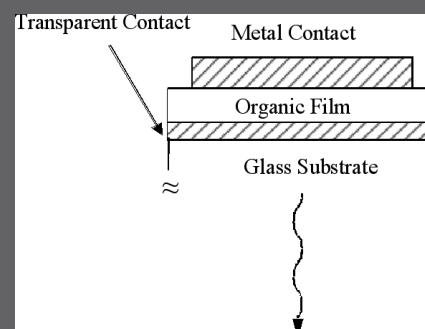


Fig. 3. Basic device structure of an organic LED.

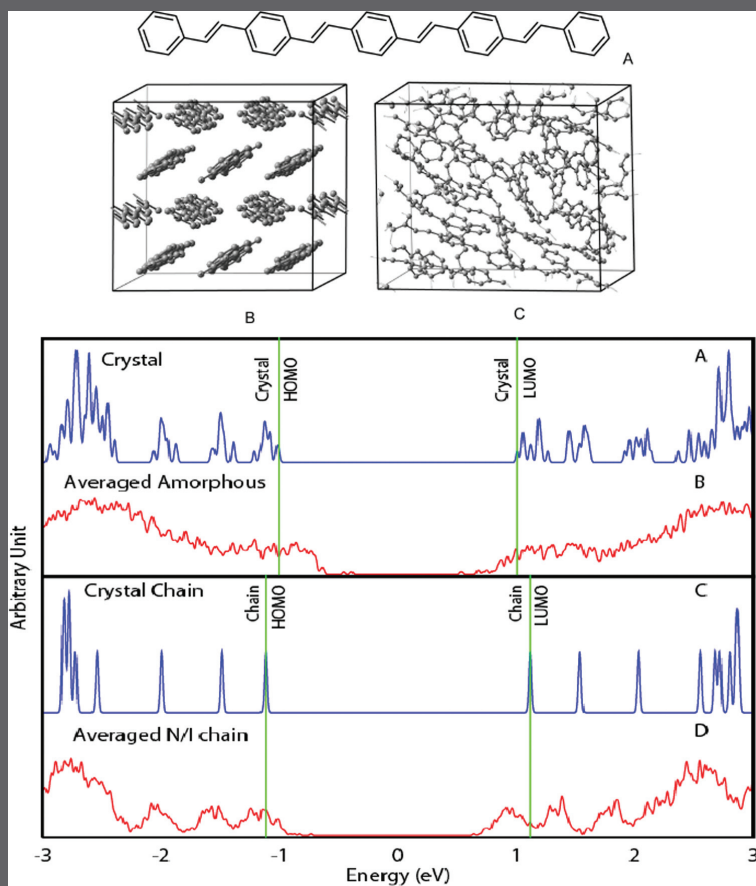


Fig. 4. Top: molecular structure of a five-ring oligomer of PPV. Middle, left: crystal structure. Middle, right: disordered structure of PPV oligomers. Bottom: calculated density of states for: A) crystal, B) disordered cluster, C) isolated ordered oligomer, and D) ensemble of isolated disordered oligomers. From [1].

the other conducting contact. The electrons and holes recombine in the organic semiconductor, emitting light whose color is determined by the energy gap of the organic semiconductor. The conducting contacts have different work functions—a high work function contact to inject holes, and a low work function contact to inject electrons. One of the conducting contacts must be transparent to let the light out of the structure, and indium tin oxide is often used for this purpose.

In our experiment's collaboration with colleagues from MPA division (Ian Campbell and Brian Crone), we are studying the basic properties of organic semiconductor devices such as LEDs. We investigated the role of intra-molecular conformational disorder and inter-molecular electronic interactions on the electronic structure of disorder clusters of (PPV) oligomers. Classical molecular dynamics was used to determine probable molecular geometries, and first-principle density functional theory (DFT) calculations were used to determine electronic structure. Intra-molecular and inter-molecular effects were disentangled by contrasting results for densely packed oligomer clusters with those for ensembles of isolated oligomers with the same intra-molecular geometries. We found that electron trap states are induced primarily by intra-molecular configuration disorder, while the hole trap states are generated primarily from inter-molecular electronic interactions. Figure 4 shows an example of these calculations, which was recently published [1].

Organic semiconductors have proven to be technologically valuable for a number of applications. Although the device details depend on the envisioned application, the basic physical processes involved do not. Therefore, a fundamental understanding of the physical processes that take place in organic semiconductors is important for a wide variety of applications. The most developed technological application of organic semiconductors at this time is displays. Figure 5 shows a flat panel TV made from organic LEDs that Sony has just introduced to the commercial market.

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[1] P. Yang et al., *Phys. Rev. B*, **76**, 241201R (2007).

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Fig. 5. Flat panel TV made from organic LEDs. Manufactured by Sony.